Sampling algorithms for generalized model ensembles in multifidelity uncertainty quantification

Workshop on Multilevel and multifidelity samplng methods in UQ for PDEs, Erwin Schrödinger Institute (Virtual)
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joint work with Gianluca Geraci, Mike Eldred and John Jakeman (SNL)

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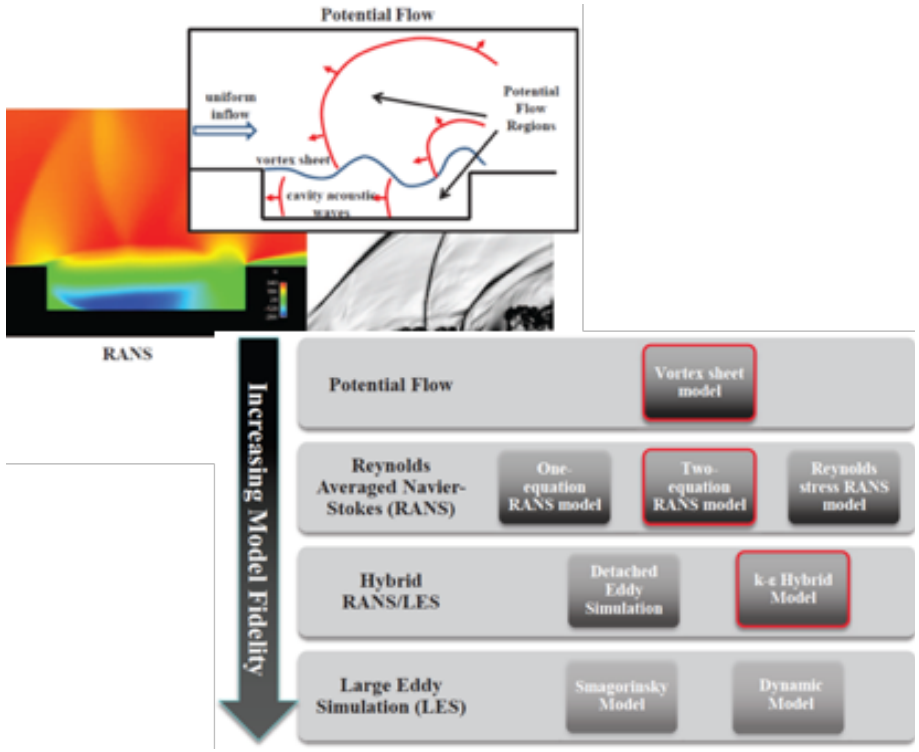
Uncertainty quantification with multiple models

Motivation

Observation: Many models and simulations are created over the course of analyzing a system.

Key idea: Usually, these models serve to **develop** the ***eventual*** high-fidelity model. How do we use them to also **analyze** the eventual high-fidelity model?.

- Information sources
  - Hierarchy of fidelities
  - Ensemble of peer models
  - Discretization levels
  - Experimental data



High-level modeling questions

1. How do we model the multi-fidelity uncertainty quantification problem?
   - How is each simulation related? (Discretization hierarchies, physics hierarchies, "competing" peers (model selection), combination)
   - How are relationships between models represented/exploited? (discrepancies, statistical correlations, probabilistic conditional dependencies, something else?)

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   - Variance/Bias reduction, MSE reduction (Frequentist)
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2. What are the algorithmic objectives of multi-fidelity uncertainty quantification?
   - Variance/Bias reduction, MSE reduction (Frequentist)
   - Probabilistic predictions (Bayesian)
3. Are there any *general* approaches for addressing these modeling questions, which can then be adapted to specific cases?

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   - How can chaotic systems be considered?
4. Simulation models have different inputs
   - Extremely common in variety of physics domain where lower fidelities replace "physics" with "models"
   - Each low-fidelity may have its own set of uncertain model parameters, while all share uncertain environmental parameters (e.g., boundary conditions)

This talk

Dealing with general model ensembles

We present several ***sampling*** approaches that avoid explicit or implicit orderings based on model fidelity or correlations.
We focus on ***variance reduction***, with some broader ideas at the end

1. Take an ***optimality and convergence*** viewpoint for variance reduction: What is the best possible performance when increasing the information from each low-fidelity information source?

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[Gorodetsky, et. al. *MFNETS: multi-fidelity data-driven networks for Bayesian learning and prediction*, (submitted) 2020]

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2. Some commonly used existing approaches built on recursive-difference and recursive-nested estimators have limited variance reduction
   - Low-fidelity sims can be infinitely evaluated with no further variance reduction
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3. Convergent estimators can be derived

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Outline

1. Notation: Monte Carlo and control variates
2. Recursive difference (MLMC) and nested difference estimators (MFMC)
3. Convergent approximate control variates
4. Probabilistic models

Monte Carlo

1. z: input parameter uncertainties
2. Q: quantity of interest evaluation

$$\hat{Q}(\boldsymbol{z}) = \frac{1}{N}\sum_{i=1}^{N} Q(z^{(i)})$$

3. The estimator is unbiased

$$\mathbb{E}\left[\hat{Q}(\boldsymbol{z})\right] = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}\left[Q(z^{(i)})\right] = \mathbb{E}\left[Q\right]$$

4. The estimator variance decays like $1/N$:

$$\mathbb{V}\text{ar}[\hat{Q}] = \frac{1}{N}\sum_{i=1}^{N} \mathbb{V}\text{ar}\left[Q(z^{(i)})\right] = \frac{\mathbb{V}\text{ar}[Q]}{N}$$

Linear control variate
Single additional information source

- Introduce a correlated information source $\hat{Q}_1(\boldsymbol{z})$

[Lavenberg and Welch 1981]

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- Suppose we **know** the mean of $\mathbb{E}\left[\hat{Q}_1(\boldsymbol{z})\right] = \mu_1$

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- Variance reduction effectiveness measured by correlation $\rho_1(\hat{Q}(\boldsymbol{z}), \hat{Q}_1(\boldsymbol{z}))$

$$\mathbb{V}\text{ar}[\hat{Q}^{\text{CV}}] = (1 - \rho_1^2)\mathbb{V}\text{ar}[\hat{Q}]$$

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Multiple Models

- Several additional random variables $\hat{Q}_i(\boldsymbol{z})$ with known means μ_i

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- Optimal weights are

$$\alpha = -\mathbb{C}\text{ov}[\hat{Q}, \hat{\boldsymbol{Q}}]\mathbb{C}\text{ov}[\hat{\boldsymbol{Q}}, \hat{\boldsymbol{Q}}]^{-1}$$

- Optimal reduction is (**note covariance amongst all low-fidelity sources**)

$$R^2 = \frac{\mathbb{C}\text{ov}[\hat{Q}, \hat{\boldsymbol{Q}}]\mathbb{C}\text{ov}[\hat{\boldsymbol{Q}}, \hat{\boldsymbol{Q}}]^{-1}\mathbb{C}\text{ov}[\hat{\boldsymbol{Q}}, \hat{Q}]}{\mathbb{V}\text{ar}[\hat{Q}]}$$

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- Single control variate case considered by [Pasupathy, Schmeiser, Taaffee, and Wang 2012] and [Ng and Willcox, 2014]

Multiple-model case

- Two families of recursive algorithms can be understood with this model
  - Recursive difference estimator (inner loop of MLMC and MIMC, [Giles, 2008], [Haji-Ali, Nobile, Tempone 2016])
  - Recursive nested estimator (Multifidelity Monte Carlo [Peherstorfer, Willcox, and Gunzberger 2016])
- Variance reduction of these recursive approaches do not converge to optimal control variate in the limit of infinite data
- Next: an interlude about robustness of some recursive approaches
- Eventual: Convergent and robust ACV estimators can be found

A limitation of some recursive schemes
Robustness to noise

- Stochastic ODE with payoff modeling European options (Giles 2008)

$$dS = rSdt + \sigma SdW \quad P = \exp(-r)\max(0, S(1) - 1)$$

- Euler-Maruyama for time integration at **different resolutions**
- Expectation is a telescopic sum —

$$\mathbb{E}[P_L] = \mathbb{E}[P_1] + \sum_{\ell=2}^{L} \mathbb{E}[P_i - P_{i-1}] \quad \mathbb{V}\text{ar}[P_L] = \mathbb{V}\text{ar}[P_1] + \sum_{\ell=2}^{L} \mathbb{V}\text{ar}[P_i - P_{i-1}]$$

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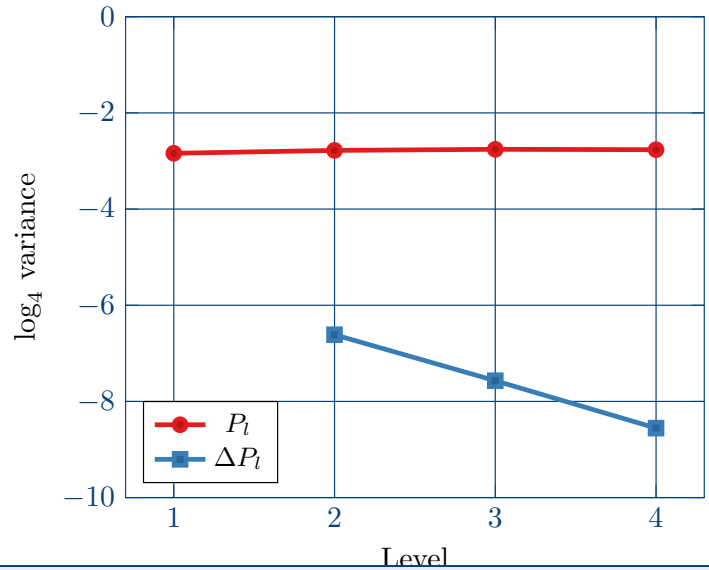
Variance Decay → MLMC



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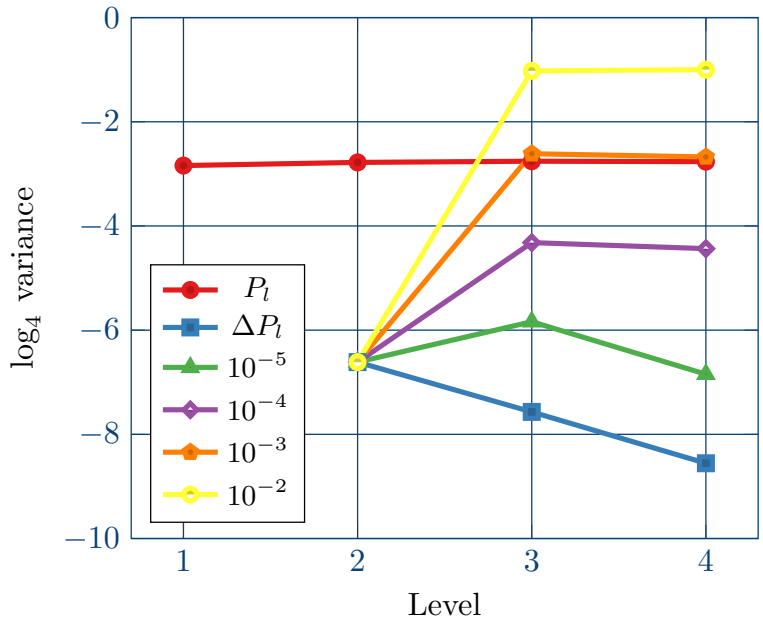
Corrupt some level 3 evals.



Recursive differences ***within*** Multilevel Monte Carlo

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$$\{Q_1, \ldots, Q_M\}$$

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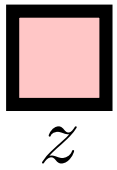

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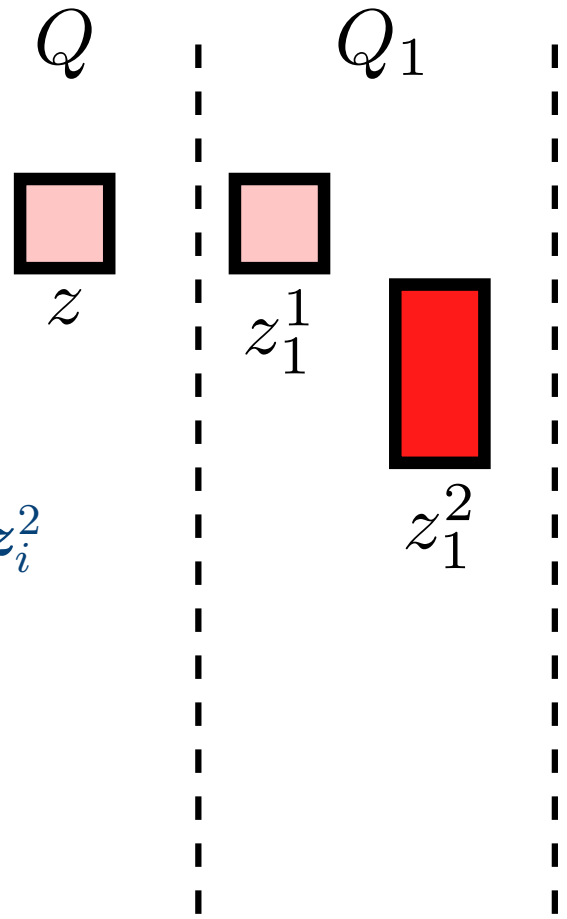

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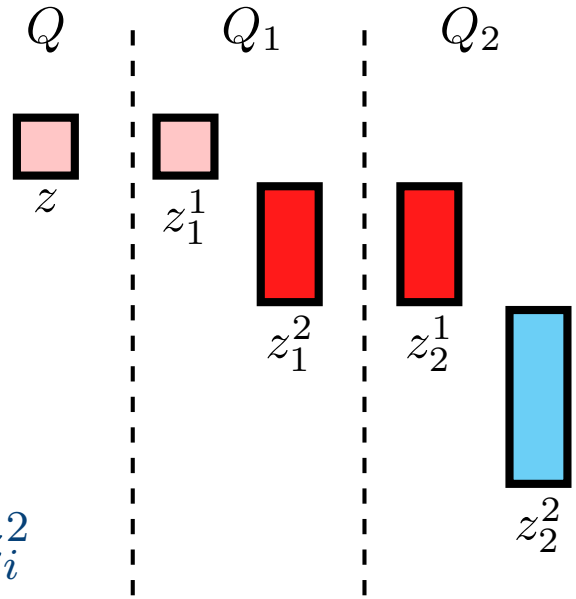

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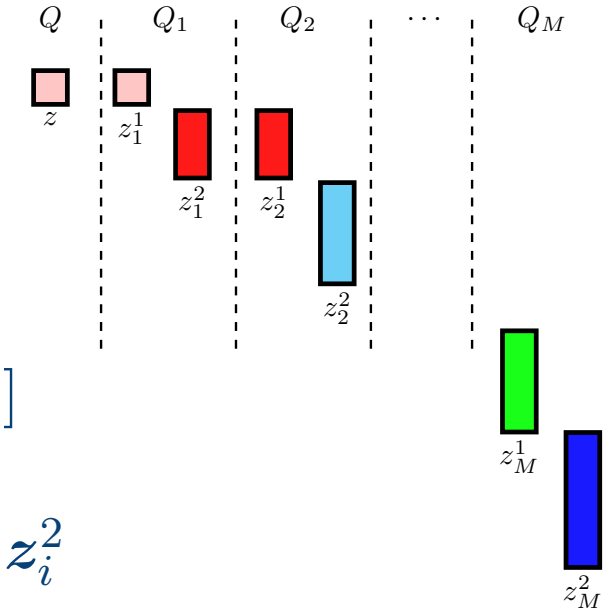

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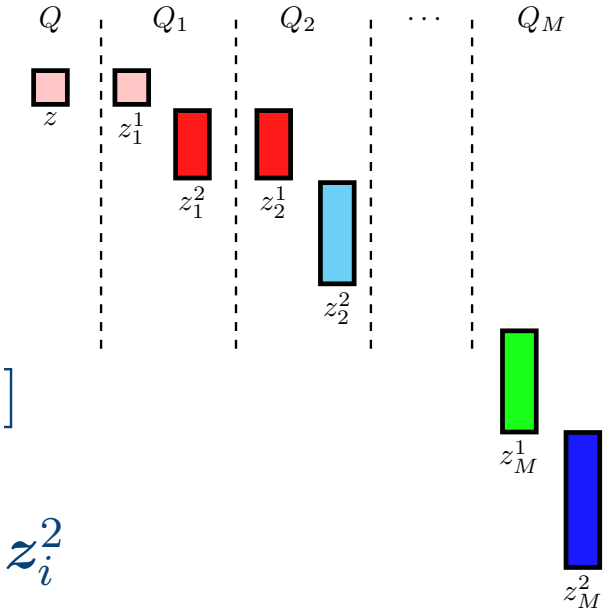

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4. This is an ACV with $\alpha = -1$ and variance

$$\mathbb{V}\text{ar}[Q] = \mathbb{V}\text{ar}[Q_L] + \sum_{\ell=L-1}^{1} \mathbb{V}\text{ar}[Q_\ell - Q_{\ell+1}] + \mathbb{V}\text{ar}[Q - Q_1]$$

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Q

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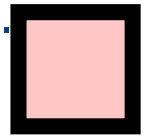

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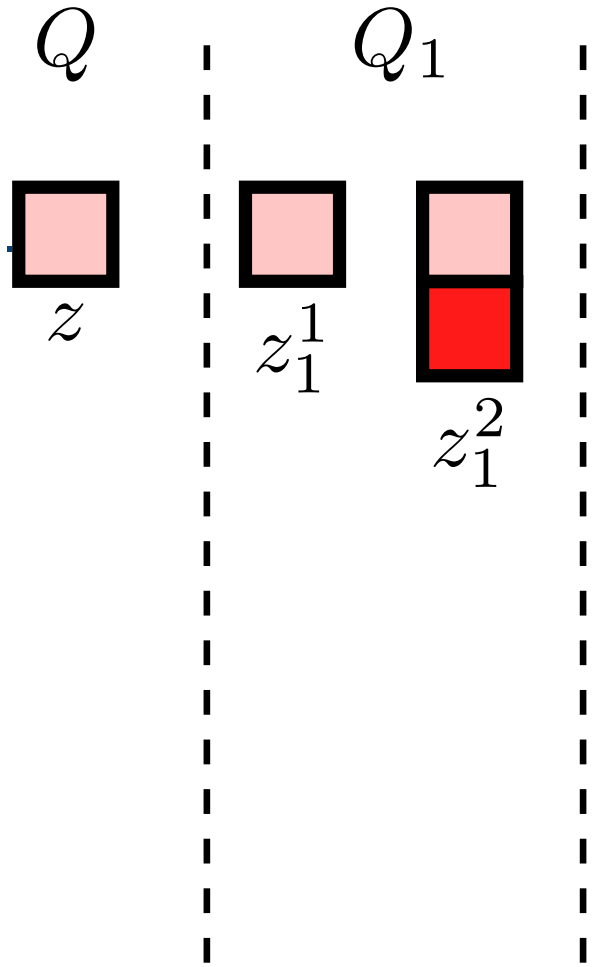

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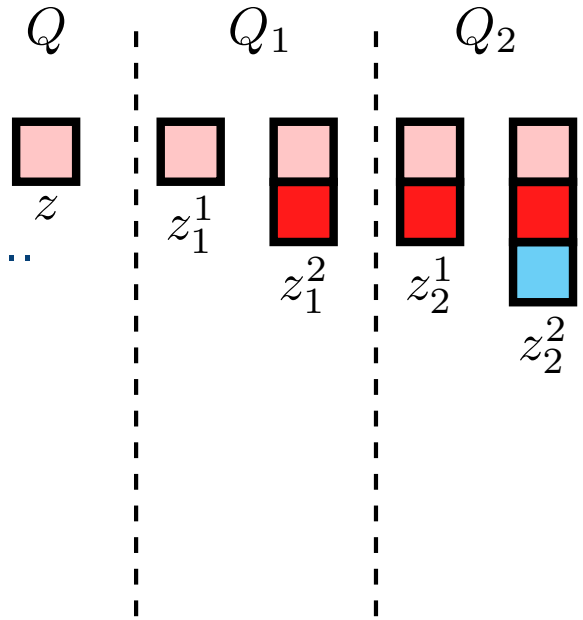

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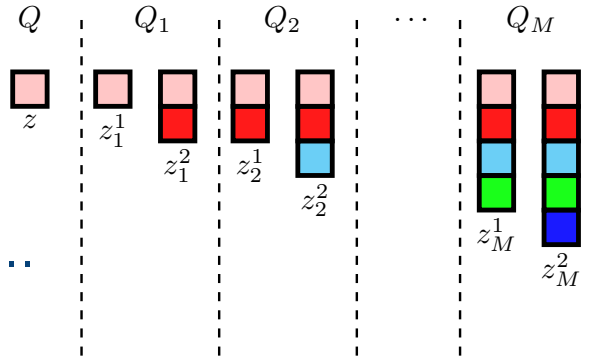

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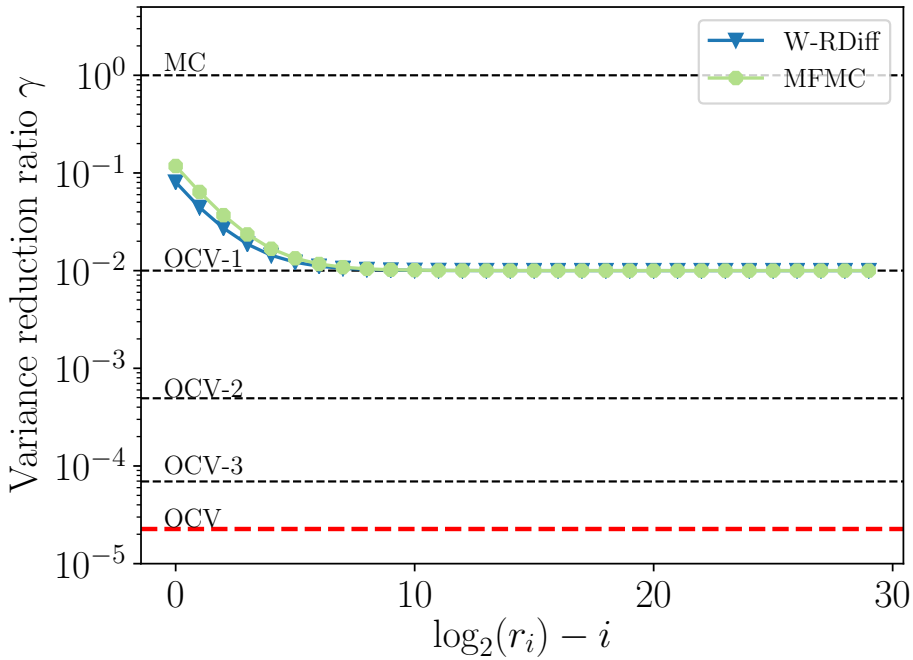
Potentially significant limitations to variance reduction

- **Fix** number of HF evaluations
- Increase the number of LF evaluations
- $Q = x^5$, $Q_1 = x^4$, $Q_2 = x^3$, $Q_3 = x^2$, $Q_4 = x$



Sub-optimality of recursive estimators

THEOREM 2.4 (Maximum variance reduction of MLMC). *The variance reduction of MLMC is bounded above by the optimal single CV i.e.,*

$$R^2_{\text{MLMC}} < \rho_1^2. \tag{2.19}$$

THEOREM 2.7 (Maximum variance reduction of MFMC). *The variance reduction of MFMC is bounded above by the optimal single CV, i.e.,*

$$R^2_{\text{MFMC}} < \rho_1^2. \tag{2.25}$$

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THEOREM 2.7 (Maximum variance reduction of MFMC). *The variance reduction of MFMC is bounded above by the optimal single CV, i.e.,*

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Why?: lack of consideration of all correlations $R^2 = \frac{\mathbb{C}\text{ov}[\hat{Q},\hat{\boldsymbol{Q}}]\mathbb{C}\text{ov}[\hat{\boldsymbol{Q}},\hat{\boldsymbol{Q}}]^{-1}\mathbb{C}\text{ov}[\hat{\boldsymbol{Q}},\hat{Q}]}{\mathbb{V}\text{ar}[\hat{Q}]}$

Sub-optimality of recursive estimators

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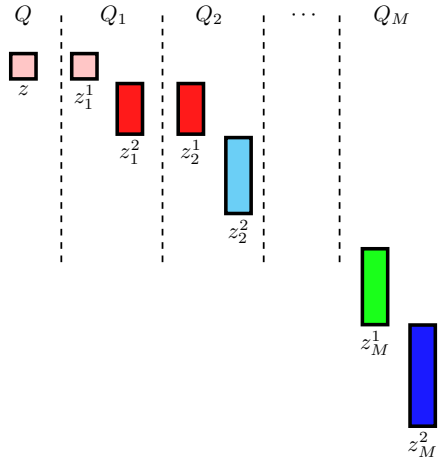
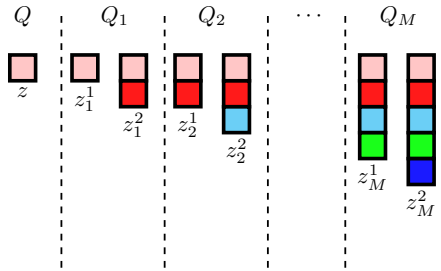
Recursive Difference



MFMC



Approximate control variates

Estimator Ansatz

$$\tilde{Q}(\boldsymbol{z}, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_M) = \hat{Q}(\boldsymbol{z}) + \sum_{i=1}^{M} \alpha_i (\hat{Q}_i(\boldsymbol{z}) - \hat{\mu}_i(\boldsymbol{z}_i^2))$$

- Ests. distinguished by distribution of samples amongst $\hat{Q}_i$ and μ_i
- Includes previous recursive estimators as specific cases

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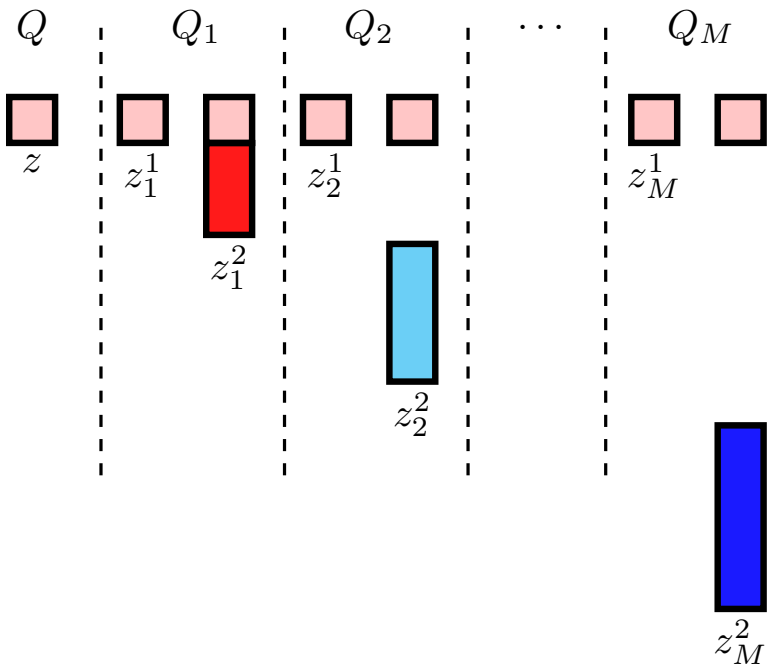
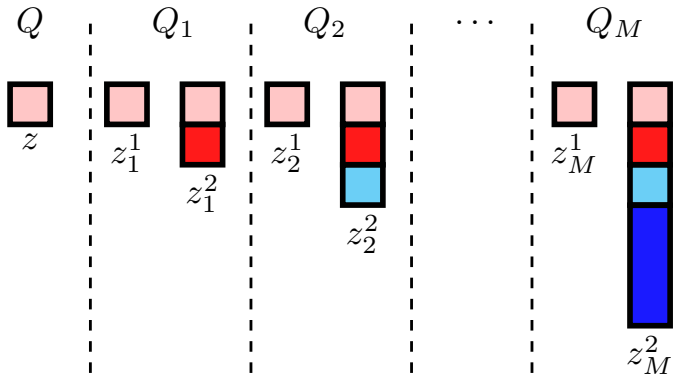
- Converges because it ***maintains correlation*** amongst all $\hat{Q}_i$

Sample allocations for two (of many) variants

Independent Samples



Shared Samples



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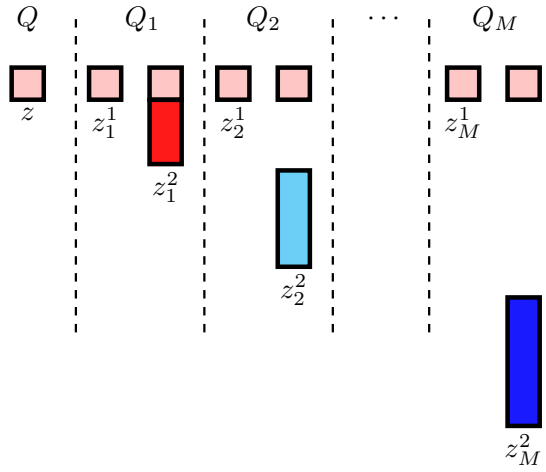
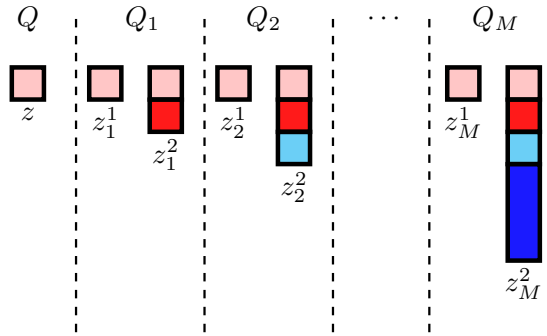


V.S.

Shared Samples



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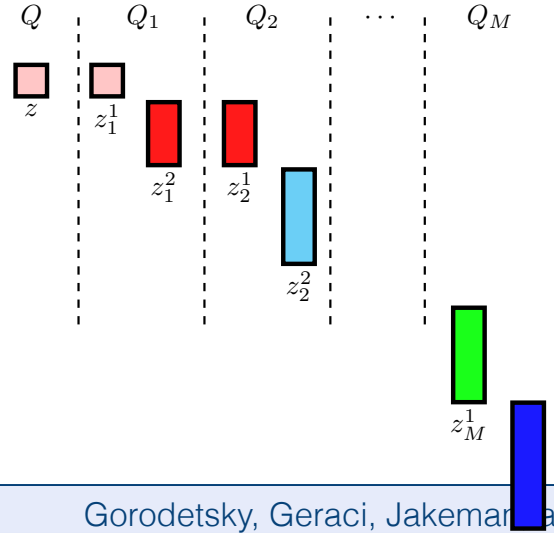
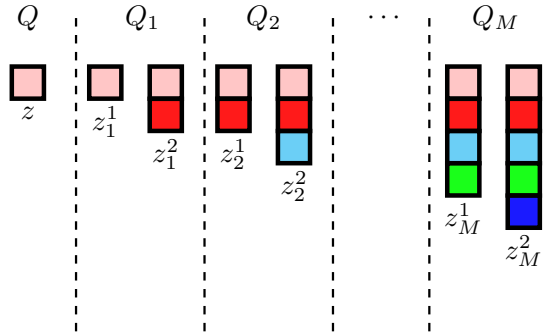
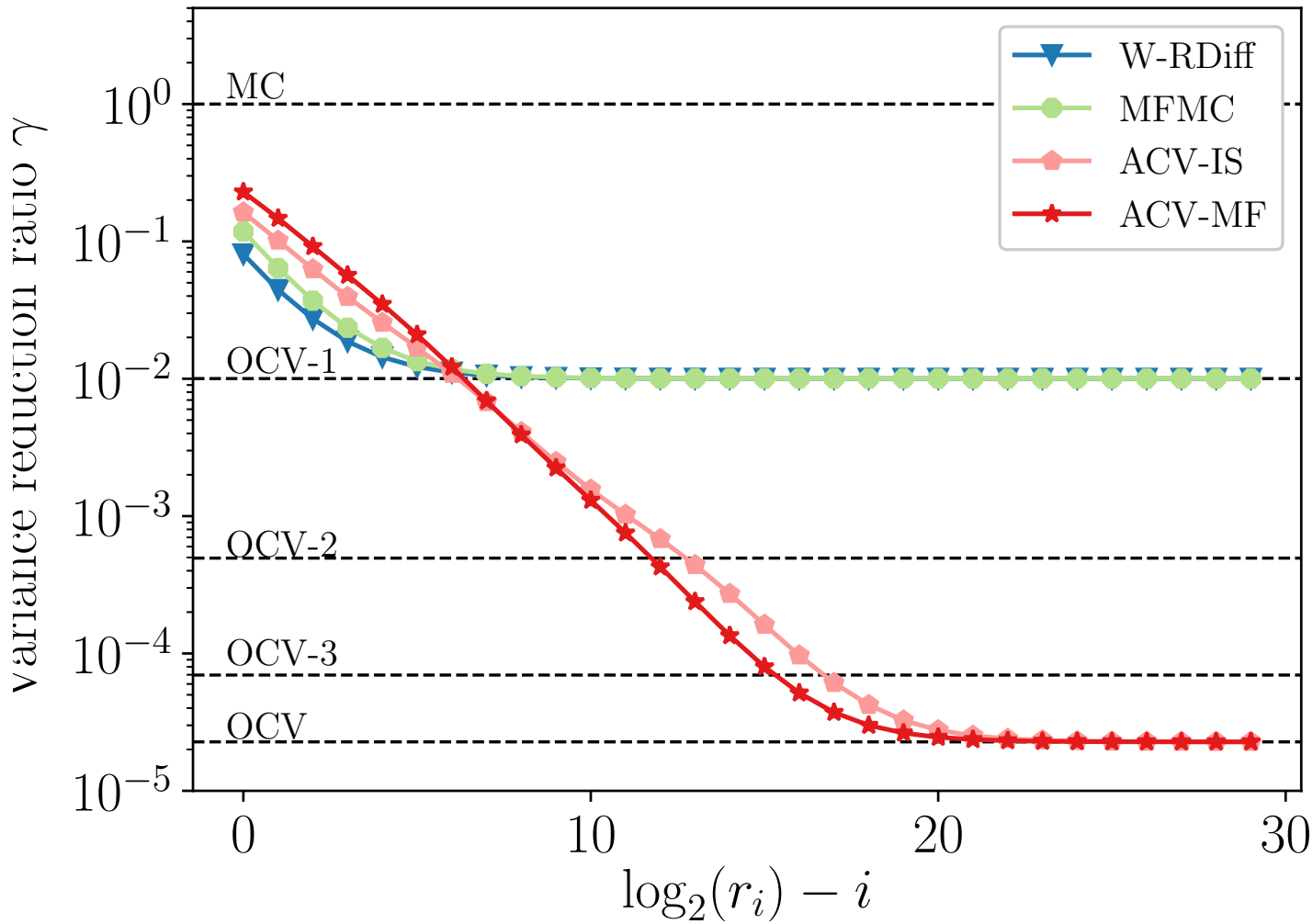


MFMC



We can prove convergence



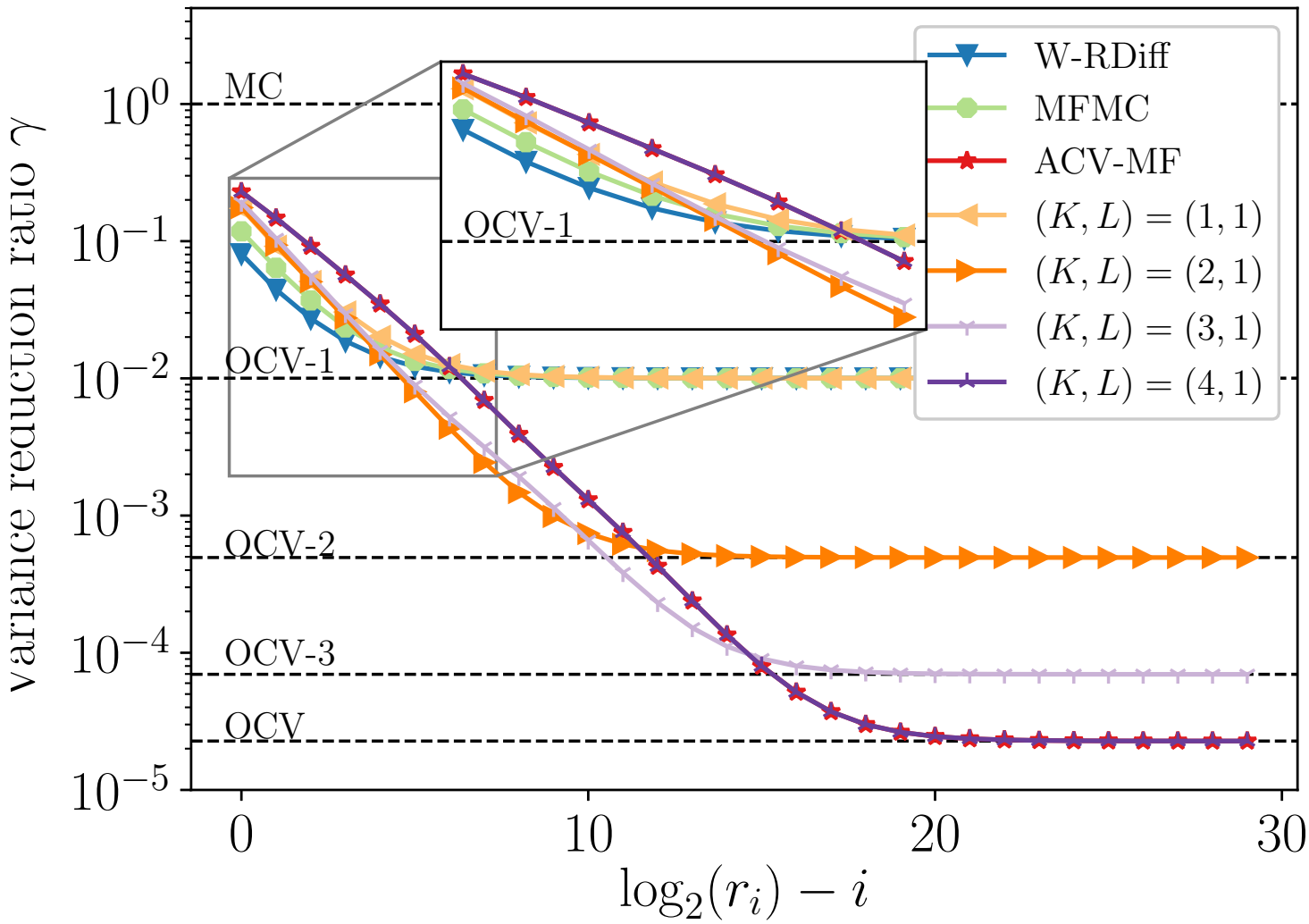
Hybrid estimator to accelerate convergence

- Use the first K control variates to accelerate the Qoi Q
- Use the last $M - K$ to accelerate the convergence of the μ_L for some L.

$$\hat{Q}^{\text{ACV-KL}}(\underline{\alpha}, \underline{\boldsymbol{z}}) = \hat{Q}(\boldsymbol{z}) + \sum_{i=1}^{K} \alpha_i \left(\hat{Q}_i(\boldsymbol{z}) - \hat{\mu}_i(\boldsymbol{z}_i) \right) + \sum_{i=K+1}^{M} \alpha_i \left(\hat{Q}_i(\boldsymbol{z}_L) - \hat{\mu}_i(\boldsymbol{z}_i) \right)$$

$$\hat{Q}^{\text{ACV-KL}}(\underline{\alpha}, \underline{\boldsymbol{z}}) = \hat{Q}_K^{\text{ACV-}MF}(\alpha_1, \ldots, \alpha_K, \boldsymbol{z}, \boldsymbol{z}_1, \ldots, \boldsymbol{z}_k) + \sum_{i=K+1}^{M} \alpha_i \left(\hat{Q}_i(\boldsymbol{z}_L) - \hat{\mu}_i(\boldsymbol{z}_i) \right)$$

Accelerated convergence to target levels



Sample Allocation

1. Optimize over distribution of samples to minimize variance for target cost

$$J_{ACV}(N, \underline{r}) = \left(1 - R^2_{ACV}\right) \frac{\mathbb{C}\text{ov}\left[Q\right]}{N}$$

2. This is a mixed-integer nonlinear program (MINLP) where N is a non-categorical integer variable, $r_i N$ are derived integer quantities, and, in the case of ACV-KL, (K, L) are categorical integer variables.

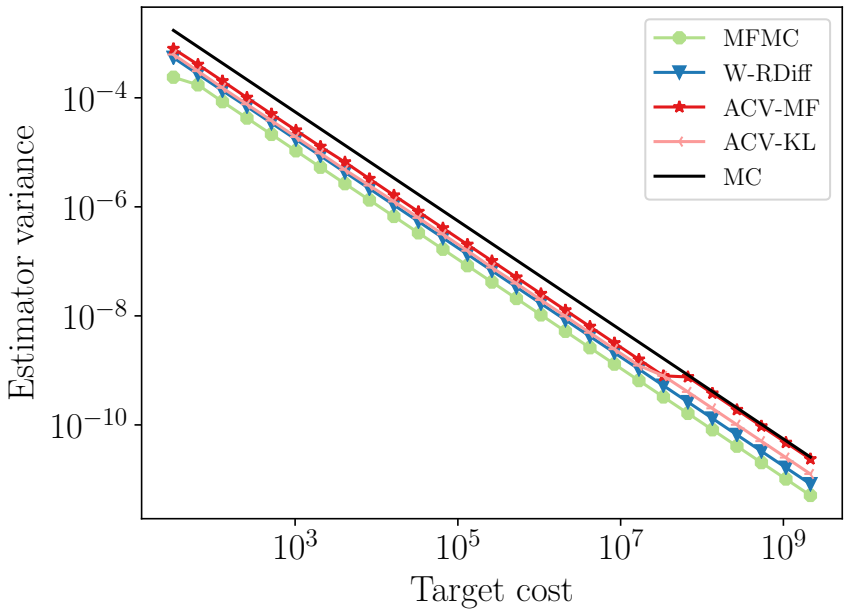
$$\min_{N,\underline{r},K,L} \log(J_{ACV}(N, \underline{r}, K, L)) \quad \text{subject to}$$

$$N\left(w + \sum_{i=1}^{M} w_i r_i\right) \leq C, \quad N \geq 1, \quad r_1 \geq 1, \text{ and } r_i \geq r_{i-1} \text{ for } i = 2, \ldots, M$$

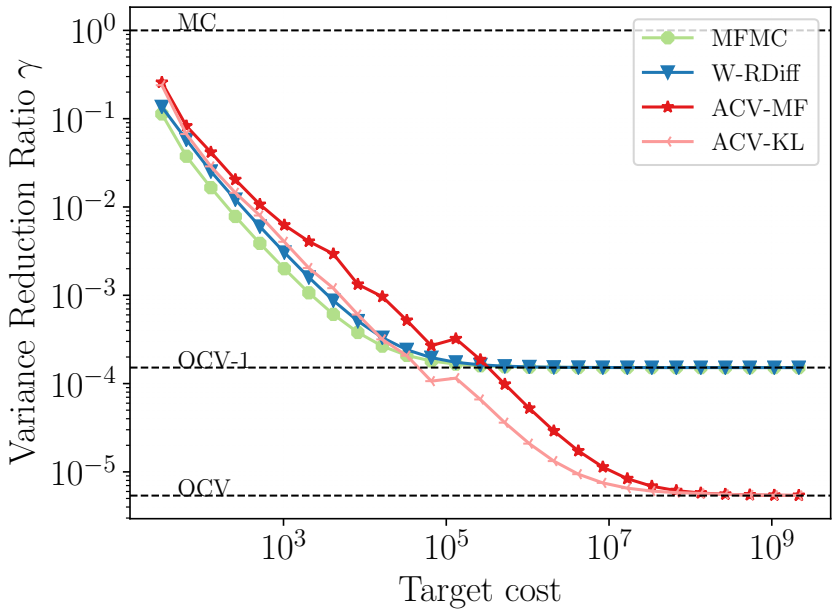
Viscous Burgers with uncertain boundaries

- Compare recursive-difference, MFMC, and optimal ACV
- Viscous Burgers at 6 discretization levels
- Estimate mean of u at a spatial location

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \kappa\frac{\partial^2 u}{\partial x^2} = 0$$

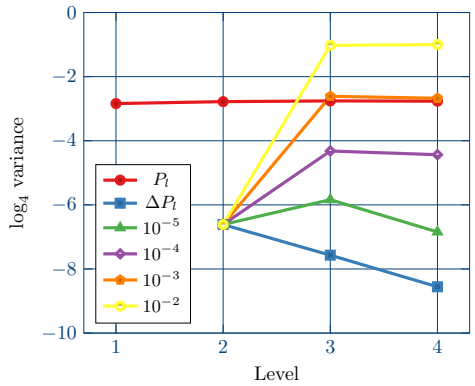


(a) Number of high-fidelity is variable

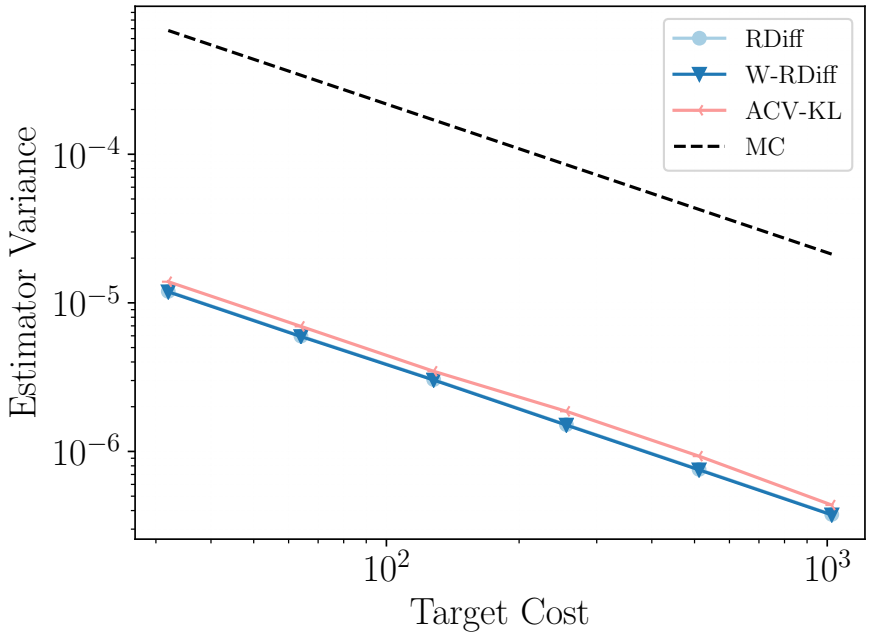


(b) Number of high-fidelity is fixed

Back to the robustness issue
Considerable improvement by using full correlations



No Corruption



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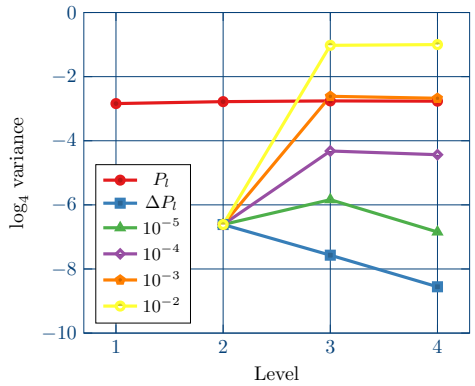
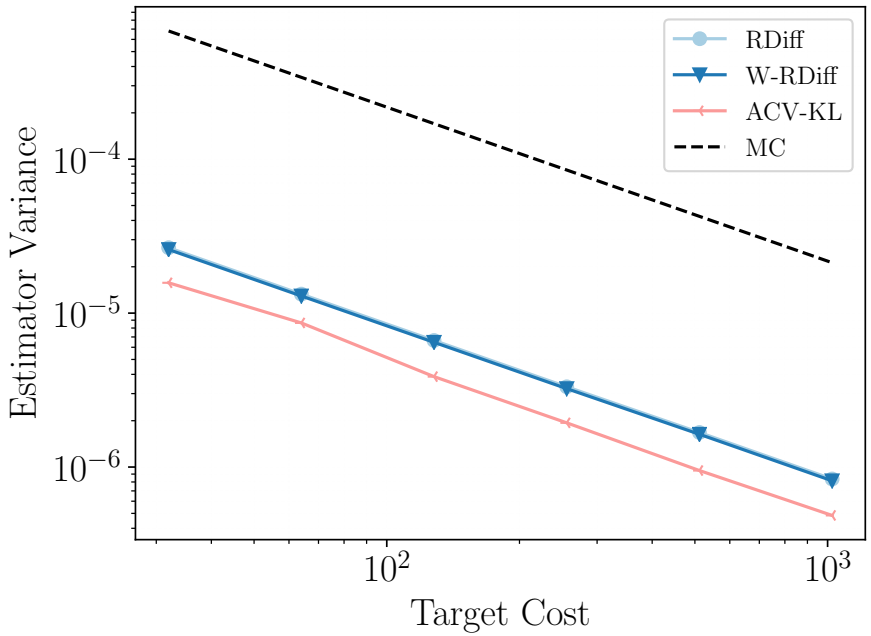


Corruption Rate: 10^{-5}



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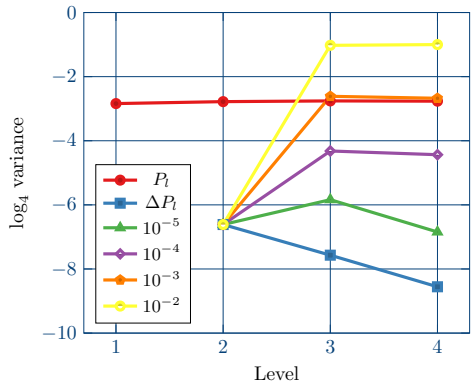
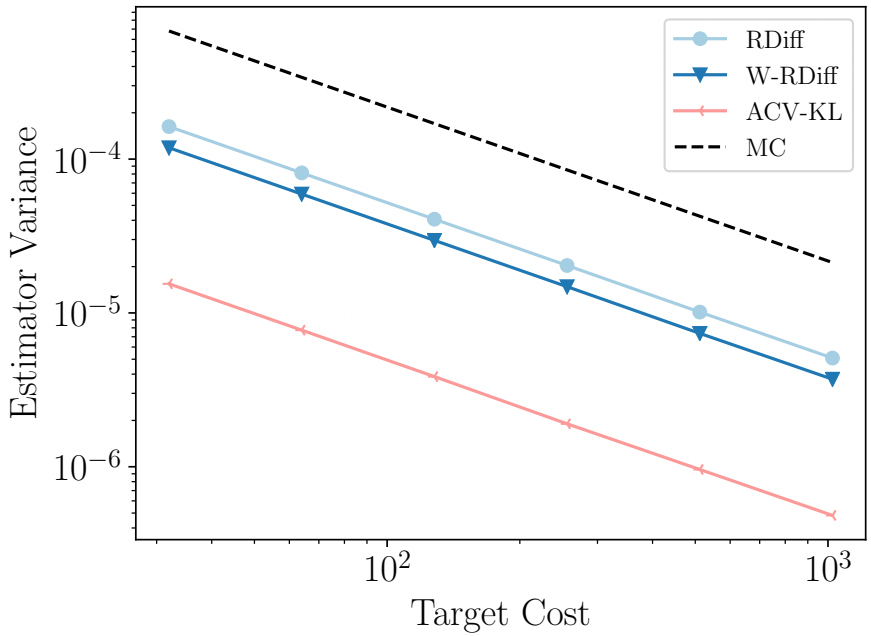


Corruption Rate: 10^{-4}

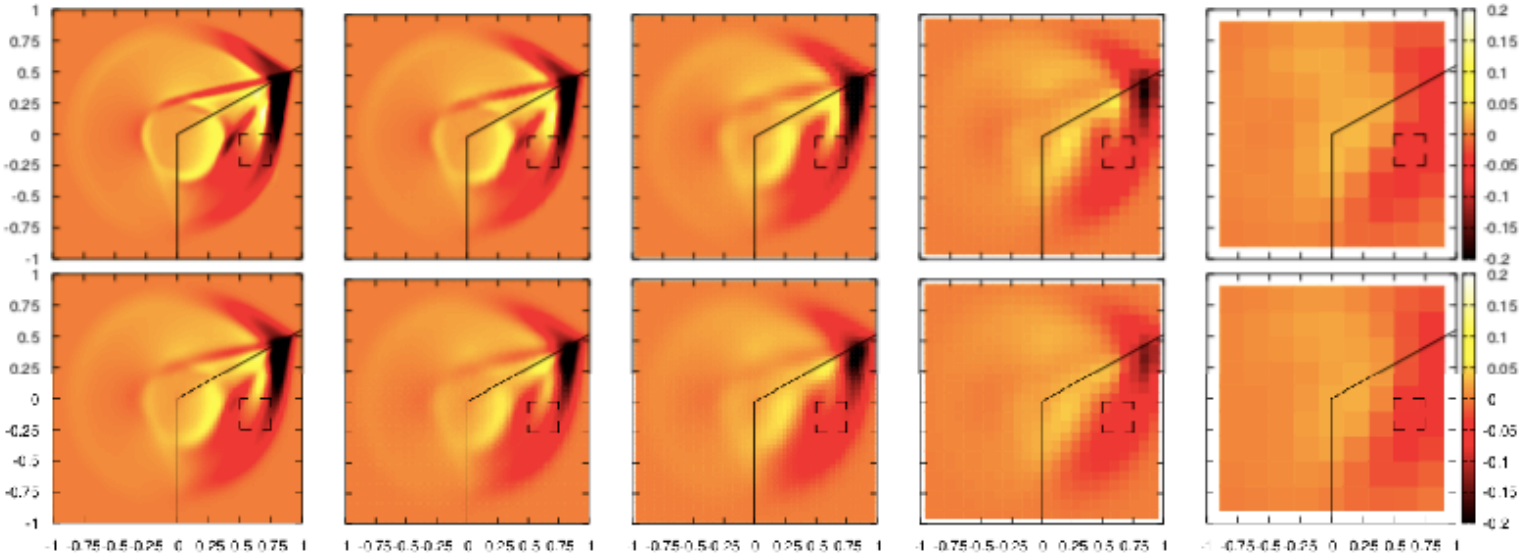


Elastic wave equation

Hyperbolic equations

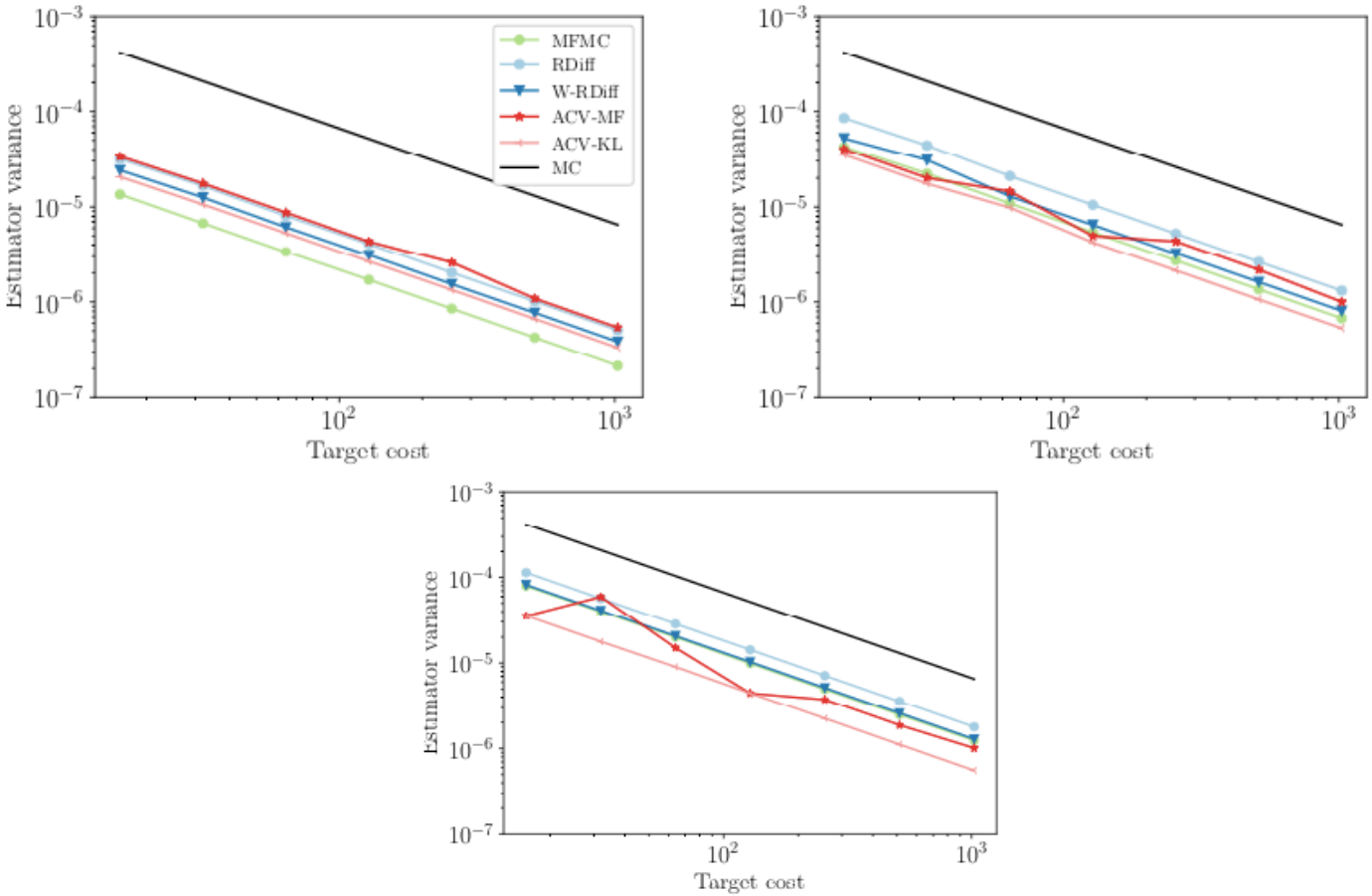
- Elastic wave propagation in two dims. with two materials
- Two numerical schemes, each scheme has different discretizations (10 total simulations)
  - Schemes: High-res second-order scheme, and first-order Godunov scheme
  - Discretizations: 200×200, 100×100, 50×50, 25×25, 10×10

$$q_t + A(q)q_x + B(q)q_y = 0,$$



Robust to aggressive coarsening

1. Left: single-fidelity with discretization hierarchy
2. Right: multi-fidelity with discretization hierarchies
3. Bottom: multi-fidelity with aggressive coarsening



Obervations

Observations:

1. The ACV is a heuristic ansatz, but a useful one as it captures many existing methods
2. Recursive approaches often work really well, general case not always needed
3. Computational gains can be gained by imposing additional structure ***when it is there***
4. Pilot sample are needed for many algorithms, their effect is poorly studied

Alternatives

Type of question we want to answer

- Can the ACV ansatz be ***derived*** from first principles rather than obtained from intuition? (yes)

[Gorodetsky, et. al. *MFNETS: multi-fidelity data-driven networks for Bayesian learning and prediction*, (submitted) 2020]

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Modeling idea

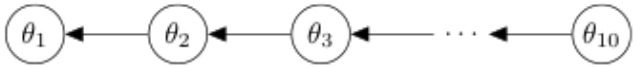
1. Parameterize a set of model relationships, then use first principle inference instead of heuristic approach
2. Will present this from a Bayesian perspective, as it provides a way to incorporate prior knowledge

[Gorodetsky, et. al. *MFNETS: multi-fidelity data-driven networks for Bayesian learning and prediction*, (submitted) 2020]

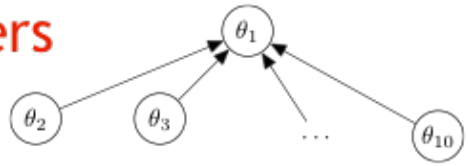
Network models

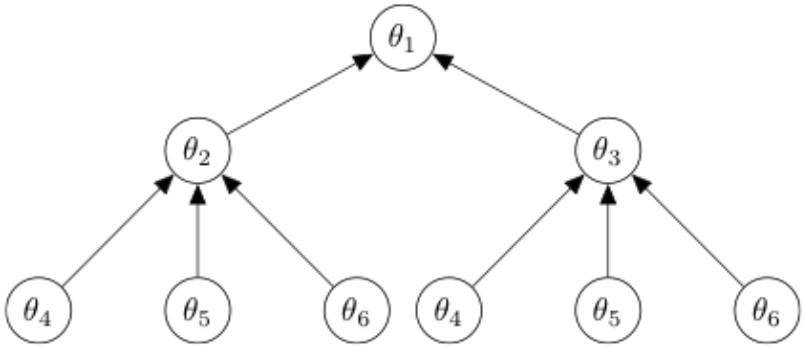
- Model multi-fidelity relationships through conditional independence relations of latent variables
- Fuse multiple models by learning their statistical relationships via network inference

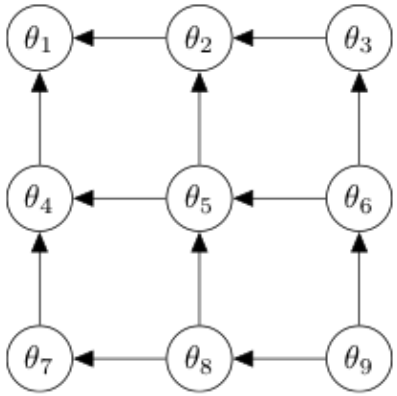
Hierarchy



Low-fidelity peers





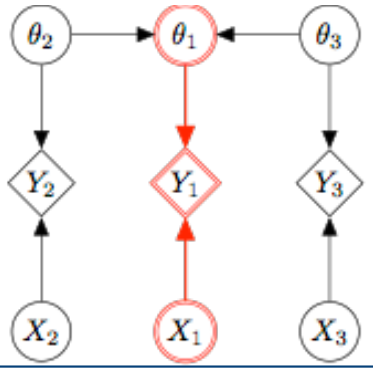


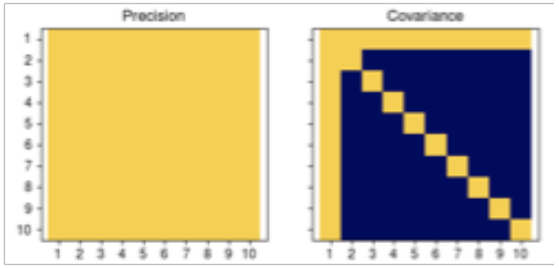
Graphs encode structure, enable scaling to many LV

Peer low-fidelity models

Example: M1 uses a composite turbulence model, M2 and 3 use components

$$p(\theta_1, \theta_2, \theta_3) = p(\theta_3)p(\theta_2)p(\theta_1|\theta_2, \theta_3)$$





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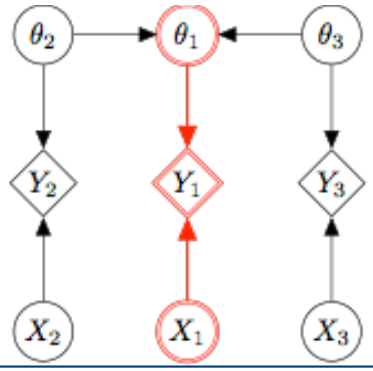

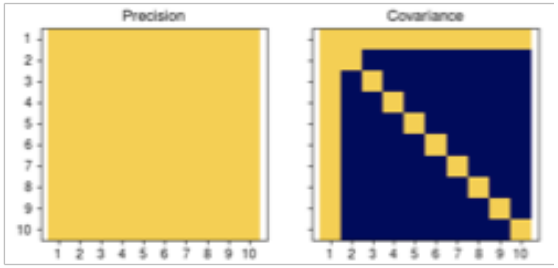

Distinct model hierarchies

Example: refined discretization as in a multilevel scheme

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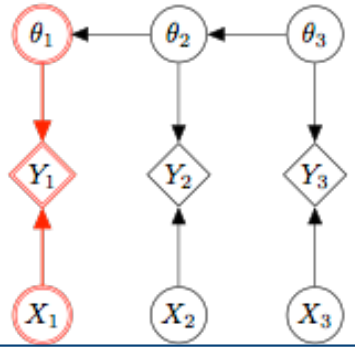

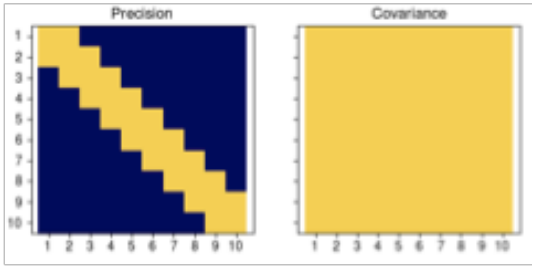

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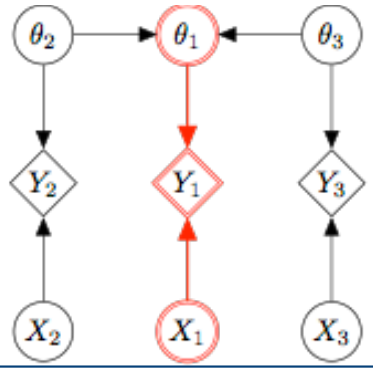

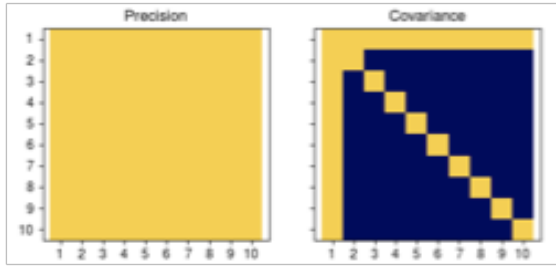

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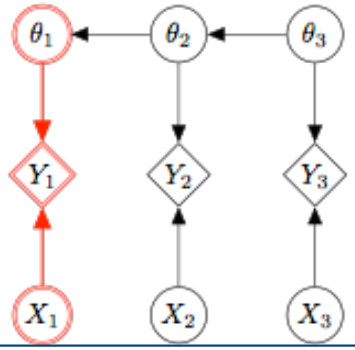

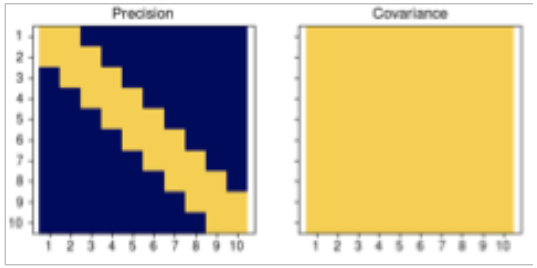

Peer high fidelity models

Example: independent high-fidelity models with an overlapping prediction

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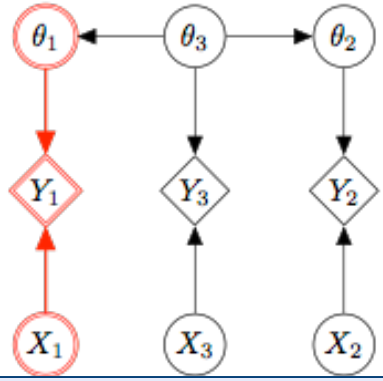

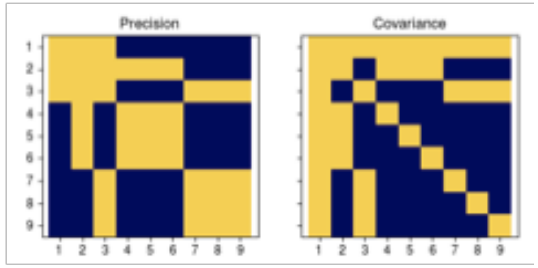

Bayesian updating and recovering control variates

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- See paper for theory where we recover CV for the general case

Back to noise robustness example

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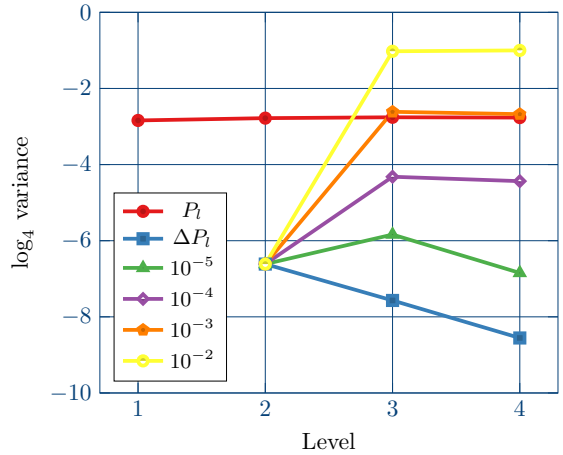
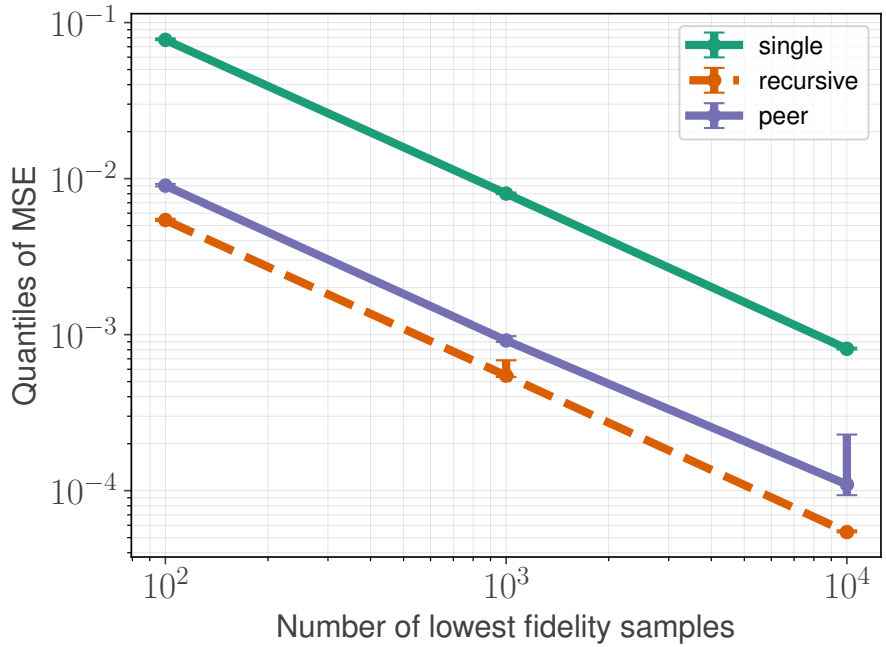


No perturbation



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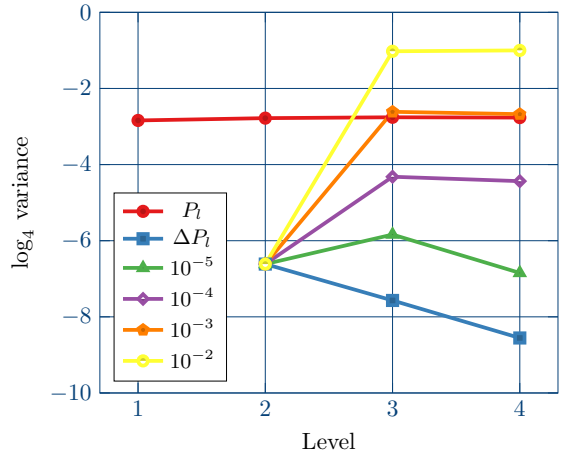
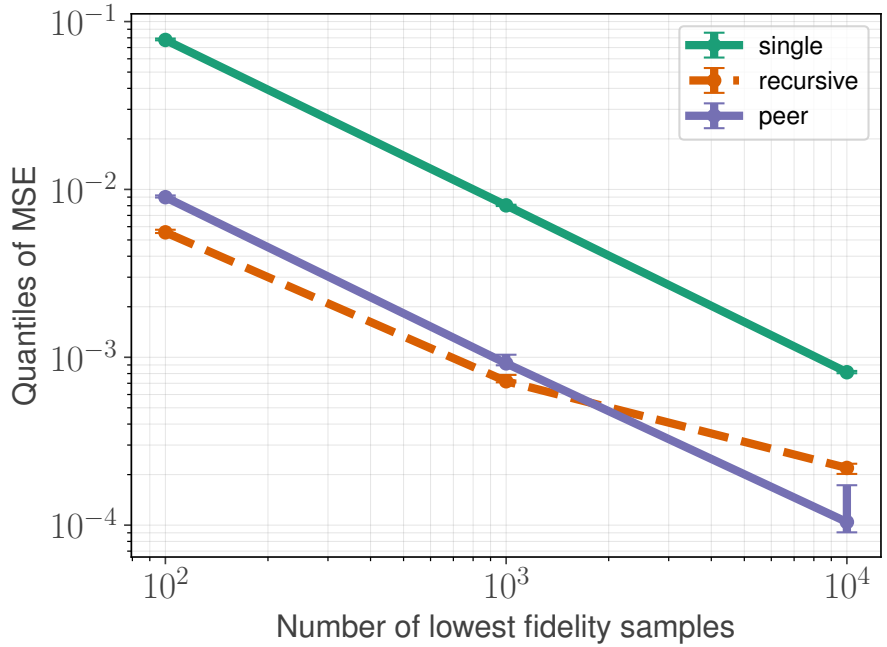


1/100 perturbation



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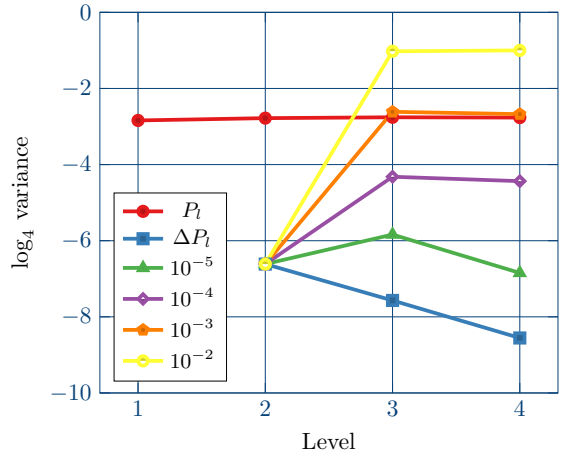

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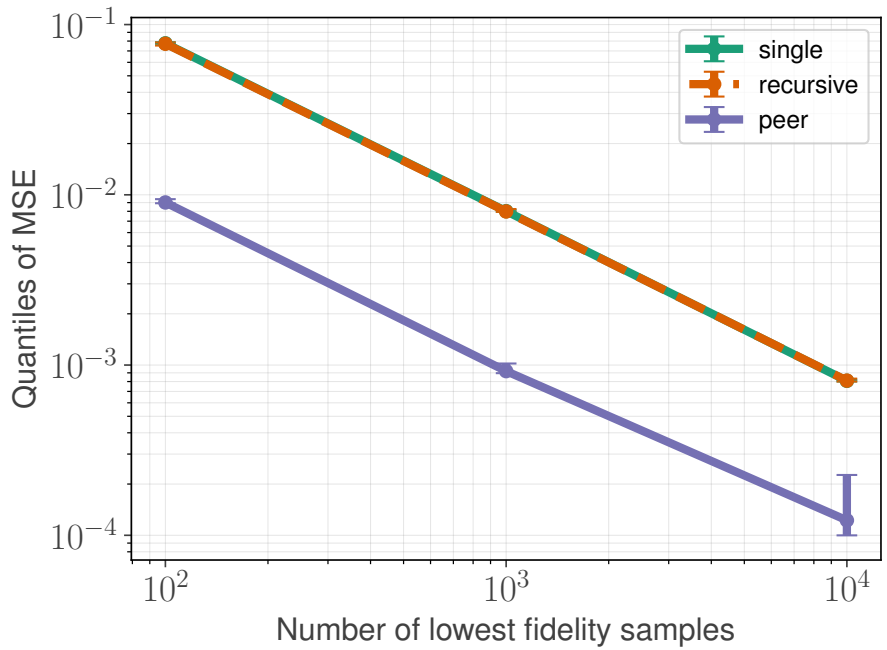

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- Papers links: see my website

  `https://www.alexgorodetsky.com/publications`

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